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Modeling jet formation around copper notch using dual domain material point method combined with molecular dynamics[1] TILAK DHAKAL, DUAN ZHANG, Los Alamos National Laboratory — Under a strong impact in metals, the material around a notch forms a jet shooting outward. We use this phenomenon as an example to test our new multi-scale computation method intended for modeling extreme material deformation and thermodynamic non-equilibrium. Starting from the Liouville equation, we derive macroscopic momentum equation with a stress tensor directly related to the molecular interactions. Such derived momentum equation can be used for thermodynamic non-equilibrium problems as long as we can calculate the stress. In cases of thermodynamic non-equilibrium, it is often difficult to obtain a constitutive relation for the stress. In this work we perform molecular dynamics (MD) simulations to calculate the stress, while the continuum level calculation is performed using dual domain material point (DDMP) method to consider extreme deformation of the material. In this multi-scale computation, each material point is a MD system. The MD systems communicate with the continuum level calculation through the strain rate and stress. An algorithm to address the extreme shear deformation in MD is developed. Since the material points do not need to communicate among each other, the MD simulations are performed in parallel in GPU using CUDA to accelerate the computation.

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